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Precise Estimates of Tunneling and Eigenvalues near a Potential Barrier

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We consider a semiclassical Schrödinger operator in one dimension with an analytic potential presenting a barrier between two potential wells. We give precise estimates for eigenvalues, eigenvalue splittings, and avoided crossings of eigenvalues near the barrier level. These estimates include bounds of the coefficients in the asymptotic expansions.

0. INTRODUCTION AND RESULTS

We consider in this paper the semiclassical Schrödinger operator in one dimension:

$$P = -h^2 \frac{d^2}{dx^2} + V(x) \text{ on } L^2(\mathbb{R}).$$

We will denote by $p = \xi^2 + V(x)$ the principal symbol of P. We will study the double-well problem at energy levels close to the top of a barrier. We make the following hypotheses on the potential $V(x)$:

(i) $V(0) = V'(0) = 0$;

(ii) $V''(0)$ is strictly negative;

(iii) $\liminf_{|x| \to \infty} V(x) > 0$;

(iv) the potential well $U = \{x \in \mathbb{R}, V(x) \leqslant 0\}$ is an interval $[-a, b]$ with $V'(-a) < 0$ and $V'(b) > 0$;

(v) V is analytic and real. (This hypothesis can be relaxed outside of a neighborhood of the well. See Remark 3.6.)

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P then has a discrete spectrum near 0 and we will consider the eigenvalue problem:

$$-h^2 \frac{d^2}{dx^2} u + V(x)u = Eu, \qquad u \in L^2(\mathbb{R}), \tag{0.1}$$

for E near 0.

The eigenvalues of (0.1) are increasing functions of h, $E_k(h)$, $k = 0, 1, \ldots$, with $E_k(h) < E_{k+1}(h)$.

In this paper we give asymptotic expansions, as h tends to 0, of eigenvalues and differences of successive eigenvalues. Many of them are well known and have been rigorously established in various papers. However, using the analyticity, we establish estimates on the coefficients in the expansions which are new as far as we know. This allows us, for example, to consider the Borel transform of the expansions or to sum them by the method of astronoms with exponentially small errors.

In order to present our results we will consider four different zones:

(1) *The Zone* $E > \varepsilon_0 > 0$. This is the one well problem. Let $E_0 > \varepsilon_0$. We recall that the difference between the first two eigenvalues larger than E_0 is of size $\pi h / T_{E_0}$, where T_E is the period of the Hamiltonian flow H_p restricted to $\{p = E\}$. If $E_{k_0}(h_0) = E_0$, the eigenvalue $E_{k_0}(h)$ is given near h_0 by the implicit equation:

$$a(E, h) = (k_0 + \tfrac{1}{2})h,$$

with

$$a(E, h) \sim \sum_{n=0}^{\infty} a_n(E) h^n.$$

Here $a_n(E)$ are analytic functions near E_0. We point out the following estimate which is new as far as we know:

There exist $C > 0$ such that near E_0: $|a_n(E)| \leqslant C^n n!$. Using a classical notion of partial differential equations we will say that $a(E, h)$ is an analytic symbol in h. (See [Sj] and the Appendix for properties of analytic symbols).

This gives the following expansion available for h small and $(k + 1/2)\pi h$ close to $a_0(E_0) = \int (\max(E_0 - V(x), 0))^{1/2}\, dx$,

$$E_k(h) \sim \sum_{n=0}^{\infty} b_n((k + \tfrac{1}{2})\, \pi h)\, h^n,$$

with the same kind of estimates as above for the functions b_n.

(2) *The zone* $E < \varepsilon_0 < 0$. This is the double-well problem. If we denote by $U(E)$ the potential well $U(E) = \{x, V(x) \leqslant E\}$, for $E < 0$, $U(E)$ is the union of two wells U_1 and U_2 and we denote by $S(E)$ the distance between these two wells for the metric $\max(V - E, 0)\,dx^2$. We show that $S(E)$ extends analytically to $E \geqslant 0$ where it becomes negative (see Proposition 2.3).

It is well known that the spectrum of P is exponentially close to the union of the spectra of P restricted to each well (See [HSj, Si]). When V is an even function of x there is a splitting of the eigenvalues which is exponentially small and of the form

$$m(E, h)\, e^{-S(E)/h} (\operatorname{mod} e^{-2S(E)/h}),$$

where $m(E, h) = (2h)/T_E + O(h^2)$ is also an analytic symbol in h (see Theorem 3.1).

In the nonsymmetric case we give also precise estimates of avoided crossings of eigenvalues. We show that the smallest difference between eigenvalues near E is of the form

$$\tilde{m}(E, h)\, e^{-S(E)/h} (\operatorname{mod} e^{-2S(E)/h}),$$

where $\tilde{m}(E, h)$ is again an analytic symbol in h with

$$\tilde{m}(E, h) = \frac{2h}{(T_{1E} T_{2E})^{1/2}} + O(h^2),$$

where T_{iE} is the period of the Hamiltonian flow H_p restricted to the well $U_i(E)$ (see Theorem 3.2).

(3) *The zone* $|E| < \varepsilon_0$ *and* $|E| \geqslant C_1 h$. (Here C_1 is some constant depending on the potential V.) In this zone, we show that there is a weak coupling of eigenvalues even above the top of the barrier (see Theorem 3.3). In the symmetric case, if we denote by E_0^+, E_0^-, E_1^+ the first successive even, odd, and even eigenvalues larger than E we have

$$\frac{1}{2}(E_1^+ - E_0^+) = \frac{\pi C_0 h}{\log(E)} + O\left(\frac{h}{\log^2(E)}\right)$$

$$(E_0^- - E_0^+) = \frac{2C_0 h}{\log(E)} \arctan((1 + O(h))\, e^{-S(E)/h}) \left(1 + O\left(\frac{1}{\log(E)}\right)\right)$$

uniformly when E and h tend to 0 in the zone 3. Here $C_0 = 2(-V''(0)/2)^{1/2}$.

(4) *The zone* $|E| < \varepsilon_0$ *and* $|E| \leqslant C_1 h$. We think that the number of k for which $|E_k(h)| \leqslant C_1 h$ is uniformly bounded in h as h tends to 0. In fact we can take C_1 of the size of C_0, say $C_1 = 2C_0$, and the number of eigenvalues trapped in this zone at h fixed is very small; we think it is less than 3.

However, we cannot analyze more precisely the difference between successive eigenvalues. We hope to come back to this problem in a later paper.

The results in the third zone were suggested to us by [FHWW] where this problem is studied for a potential $V(x)$ equal to $-\frac{1}{2}x^2$ near 0. To prove the results we construct exact solutions of (0.1) in the complex domain along the lines of Voros [V] and Ecalle [E] and we use their W.K.B. expansions. This is the so-called exact W.K.B. method. We want to thank B. Helffer for several interesting discussions and for referring us to the work of Ford, Hill, Wakeno, and Wheeler.

1. Solutions of the Schrödinger Equation in the Complex Domain

1.1. *The Exact W.K.B. Method*

In this section we recall a method due to Ecalle (see [G] and references there) to write the solution of (0.1) in a complex domain as a convergent series.

Let Ω be a simple connected open set of $\mathbb{C}$. We assume that $V(x)$ is holomorphic in Ω. We introduce the change of variables

$$z = z(x) = \int_{x_0}^{x} (V(t) - E)^{1/2}\, dt, \tag{1.1}$$

where x_0 is a base point in Ω. Here $z(x)$ is defined on the Riemann surface of $(V-E)^{1/2}$ above Ω. The points where $V(x) = E$ are called turning points and play an important role as we shall see later.

If x_0 is a simple turning point, i.e., a simple zero of $V-E$, we get

$$z(x) - z(x_0) = \tfrac{2}{3}(V'(x_0))^{1/2}(x-x_0)^{3/2}(1 + g(x-x_0)),$$

where g is holomorphic and $g(0) = 0$.

If x_0 is a double turning point, i.e., a double zero of $V-E$, we get

$$z(x) - z(x_0) = \frac{1}{2}\left(\frac{V''(x_0)}{2}\right)^{1/2}(x-x_0)^2(1 + g_1(x-x_0)),$$

with g_1 as g. We see that z is holomorphic near x_0.

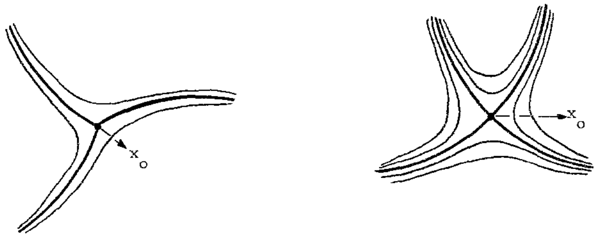
In both cases it is easy to get the picture of Stoke lines (resp. anti-Stokes lines) near x_0, which are lines along which $\operatorname{Re} z(x)$ (rèsp. $\operatorname{Im} z(x)$) is constant (see Sibuya [S]).

In Fig. 1.1 we draw only the Stokes lines. (The anti-Stokes lines are orthogonal to them.)

The Stokes lines starting from x_0 have argument

$\pi/3 - \frac{1}{3}\operatorname{Arg} V'(x_0) \bmod 2\pi/3$ if x_0 is simple and

$\pi/4 - \frac{1}{4}\operatorname{Arg} V''(x_0) \bmod \pi/2$ if x_0 is double.



simple turning point double turning point

FIGURE 1.1

The situation near a simple turning point is stable, but if we change E or V a little the double turning point may split into two ones as shown in Fig. 1.2. With $u(x) = (V-E)^{-1/4} f(z(x))$, an elementary computation shows that equation (0.1) becomes

$$-f'' + \left(H^2 - H' + \frac{1}{h^2}\right) f = 0, \tag{1.2}$$

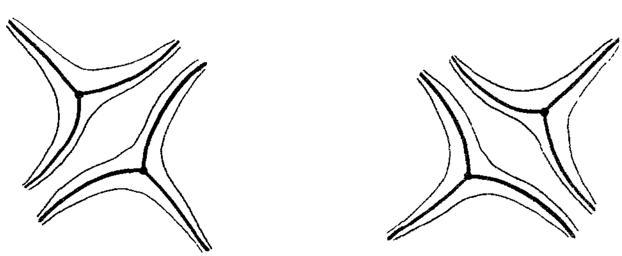
where $H(z(x)) = -\frac{1}{4}(V(x)-E)^{-3/2} V'(x)$. If x_0 is a turning point of order n (a zero of order n of $V-E$), near $z_0 = z(x_0)$, H is of the form

$$H(z) = -\frac{1}{4} \frac{n}{(n/2)+1} \frac{1}{(z-z_0)} \left(1 + g_n((z-z_0)^{1/((n/2)+1)})\right),$$

where g_n is holomorphic and $g_n(0) = 0$. If x_0 is a simple pole of $V-E$ this estimate stays true with $n = -1$.

We look now for solutions of (1.2) of the form

$$f_\pm(z) = e^{\pm z/h} \left(\sum_{n=0}^{\infty} W_{n,\pm}(x) \right).$$



$E > E_0$ $E < E_0$

FIGURE 1.2

Formally, we obtain the $W_{n,\pm}$ by solving the recurrent equations:

$$W_{0\pm} = 1$$
$$\left(\frac{\partial}{\partial z} \pm \frac{2}{h}\right) W_{2p+1,\pm} = -HW_{2p,\pm} \qquad (1.3)_\pm$$
$$\frac{\partial}{\partial z} W_{2p,\pm} = -HW_{2p-1,\pm}.$$

We assume that x stays in a simply connected open set $\Omega_1 \subset \Omega$ without turning points, so that H has no singularities in $z(\Omega_1)$. We choose a base point $z_1 = z(x_1)$ in $z(\Omega_1)$ and construct solutions of $(1.3)_\pm$ under the form

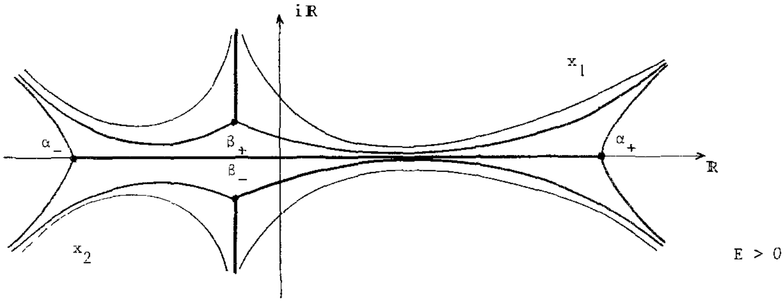
$$W_{2p+1,\pm} = -\int_{\Gamma_{2p+1}(z_1,z)} F_\pm(t,z)\, H(t_1) \cdots H(t_{2p+1})\, dt_1 \cdots dt_{2p+1}$$
$$\text{with } F_\pm(t,z) = \exp(\pm(2/h)(t_1 - t_2 + t_3 - \cdots + t_{2p+1} - z))$$
$$W_{2p,\pm} = \int_{\Gamma_{2p}(z_1,z)} G_\pm(t)\, H(t_1) \cdots H(t_{2p})\, dt_1 \cdots dt_{2p} \qquad (1.4)$$
$$\text{with } G_\pm(t) = \exp(\pm(2/h)(t_1 - t_2 + \cdots - t_{2p})).$$

Here $\Gamma_n(z_1, z)$ is the set of n-uples$(t_1, ..., t_n)$ put in increasing order on the path $\Gamma(z_1, z)$. If $\sup_{\Gamma(z_1,z)} |e^{\pm 2t/h} H| \leqslant A$ and length $(\Gamma) \leqslant L$ we easily get $|W_{p,\pm}(z)| \leqslant C(AL)^p/p!$, so that the series $\sum_0^\infty W_{n,\pm}(z)$ are convergent. However, to get asymptotic expansions in h for the $W_{n,\pm}$, we must take the path $\Gamma(z_1, z)$ such that $\pm \operatorname{Re} t$ is strictly increasing along $\Gamma(z_1, z)$. We see that the path $z^{-1}(\Gamma(z_1, z))$ must cross the Stokes lines in increasing order (resp. decreasing order).

Some Stokes lines of (0.1) are indicated on Fig. 1.3, for $E > 0$ and $E < 0$. We denote by $f_\pm(x_0, x_1, z)$ the solution of (1.2) obtained with base points x_0, x_1 in (1.1), (1.4). We will also note

$$\psi_\pm(z_1, z, h) = \sum_0^\infty W_{2p,\pm}(z, h)$$
$$\varphi_\pm(z_1, z, h) = \sum_0^\infty W_{2p+1,\pm}(z, h). \qquad (1.5)$$

It is important to notice that the functions we constructed are exact solutions of (0.1), defined, for example, everywhere on $\mathbb{R}$, even if the expressions obtained are defined only on the Riemann surface of $(V - E)^{1/2}$.



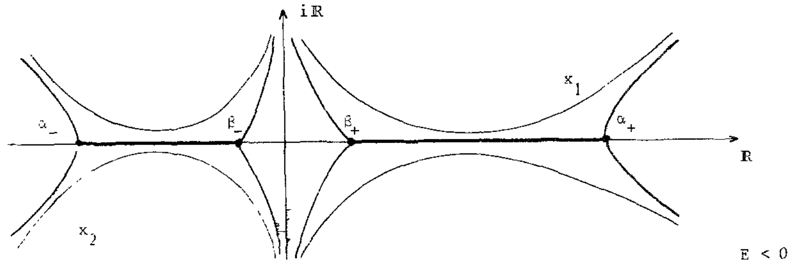


FIGURE 1.3

1.2. *The Wronskians*

We now compute the Wronskian of two solutions of (0.1) obtained as above. Recall that if u, v are two solutions of (0.1), the Wronskian $W(u, v)(x_0) = u(u_0)\, v'(x_0) - u'(x_0)\, v(x_0)$ is zero if and only if u and v are collinear, and is independent of x_0, in view of the absence of first derivatives in (0.1).

PROPOSITION 1.1. *Denote by* $u_+(x_0, x_1, x, h)$, $u_-(x_0, x_2, x, h)$ *two solutions of* (0.1) *obtained as above using* $f_+(x_0, x_1, z)$ *and* $f_-(x_0, x_2, z)$. *Then* $W(u_+, u_-) = W(f_+, f_-) = -(2/h)\psi_+(z_1, z_2, h)$.

Proof. We take the same determination of $(V-E)^{1/4}$ (hence of $(V-E)^{1/2}$) on Ω_1 for u_+ and u_-. An easy computation shows that

$$W_x(u_+, u_-) = \left((V-E)^{1/4} u_+ \frac{df_-}{dz} - (V-E)^{1/4} u_- \frac{df_+}{dz}\right)(z) = W_z(f_+, f_-).$$

Using that $f'_\pm(z) = e^{\pm z/h}(\pm(1/h)(\varphi_\pm + \psi_\pm) + \varphi'_\pm + \psi'_\pm)$ and the Eqs. $(1.3)_\pm$, we get

$$\begin{aligned}
W(f_+, f_-) &= -\frac{1}{h}(\varphi_- + \psi_-)(\varphi_+ + \psi_+) + \left(-H\psi_- + \frac{2}{h}\varphi_- - H\varphi_-\right)(\varphi_+ + \psi_+) \\
&\quad -\frac{1}{h}(\varphi_+ + \psi_+)(\varphi_- + \psi_-) - \left(-H\psi_+ - \frac{2}{h}\varphi_+ - H\varphi_+\right)(\varphi_- + \psi_-) \\
&= \frac{2}{h}(\varphi_+\varphi_- - \psi_+\psi_-).
\end{aligned}$$

Since $\varphi_+(z_1) = \varphi_-(z_2) = 0$, $\psi_+(z_1) = \psi_-(z_2) = 1$, if we compute $W(f_+, f_-)$ at z_2, we get $W(f_+, f_-) = -(2/h)\,\psi_+(z_2)$, which completes the proof. ▌

PROPOSITION 1.2. *The functions $\varphi_\pm(z_1, z, h)$, $\psi_\pm(z_1, z, h)$ are classical analytic symbols in h of order* 0, *for* $\operatorname{Re} z$ *bigger than* $\operatorname{Re} z_1$.

Proof. In the Appendix, it is shown that the recurrent Eqs. $(1.3)_\pm$ can be solved formally in the class of analytic symbols and that the formal sum $\sum_0^\infty \tilde{W}_{n,\pm}(z, h)$ is also an analytic symbol.

To finish the proof we estimate first the integral:

$$I(f, h) = \int_{z_0}^{z} e^{(2/h)(t_1 - z)} f(t_1)\, dt_1.$$

Using Taylor's formula at z and the change of variables $s = (t_1 - z)/h$, we get

$$\begin{aligned}
I(f, h) &= \int_{(z_0 - z)/h}^{0} e^{2s}\left(f(z) + shf'(z) + \cdots + s^n \frac{h^n}{n!} f^{(n)}(z)\right)h\, ds \\
&\quad + \int_{(z_0 - z)/h}^{0} e^{2s} s^{n+1} h^{n+2} g(hs + z_0)\, ds \\
&= \sum_{|\alpha| \leqslant n} c_\alpha(z, f) h^\alpha + O(h^{n+1}). \qquad (1.6)
\end{aligned}$$

Equation (1.6) immediately shows by recurrence that the $W_{n,\pm}(z, h)$ have the $\tilde{W}_{n,\pm}(z, h)$ as asymptotic expansions.

It remains to prove that, for example, ψ_+ has $\sum_0^\infty W_{2p,+}(z, h)$ as asymptotic expansion. To do that, we use (1.6) for $n = 0$. If Ω is a neighborhood of z containing the paths $\Gamma(z_0, \tilde{z})$ for $\tilde{z} \in \Omega$, we get

$$\sup_\Omega |I(f)| \leqslant Ch(\sup_\Omega |f| + h \sup_\Omega |f'|).$$

If we put $\|f\| = \sup_\Omega |f| + h \sup_\Omega |f'|$, using the fact that $I'(f) = \frac{1}{2}I(f) + f$, we get

$$\|I(f)\| \leqslant Ch\, \|f\|. \qquad (1.7)$$

If we estimate now the integral $J(f)=\int_{z_0}^{z} f(t_1)\,dt_1$, it is clear that $\|J(f)\| \leqslant C\,\|f\|$.

Since $W_{2n+1}=I(-HW_{2n})$ and $W_{2n}=J(-HW_{2n-1})$ we obtain the estimate

$$\begin{aligned} \|W_{2n+1}\| &\leqslant C_0(Ch)^n \\ \|W_{2n}\| &\leqslant C_0(Ch)^n. \end{aligned} \tag{1.8}$$

It is clear that $\psi_+ - \sum_{p=0}^{N} W_{2p,+}(z,h)$ is $O(h^{N+1})$ for h small enough, which proves the proposition. ∎

Proposition 1.2 implies the following proposition:

PROPOSITION 1.3. *$W(u_+, u_-)$ is an analytic symbol of h, depending holomorphically on (z_1, z_2), if we can join z_1 to z_2 with a path avoiding the turning points along which* $\operatorname{Re} z$ *is strictly increasing.*

2. The Eigenvalue Equation

2.1. *Particular Solutions of* (0.1)

We apply now the method of Section 1 to our problem.

We take for Ω a complex neighborhood of $\mathbb{R}$, contained in the domain of holomorphy of V. If Ω is small enough and E is near 0 but different from 0, there are exactly four simple turning points for $(V-E)$ in Ω, $\alpha_\pm(E)$ and $\beta_\pm(E)$ (see Fig. 1.3).

— $\alpha_\pm(E)$ is the positive (resp. negative) zero of $V-E$ which stays away from a neighborhood of 0.

— $\beta_\pm(E)$ are the two zeroes of $V-E$ near 0. If $E>0$ we put $\operatorname{Im}\beta_+(E)>0$, $\operatorname{Im}\beta_-(E)<0$, and if $E<0$ we put $\beta_+(E)>0$, $\beta_-(E)<0$.

It is easy to check that the Stokes lines for $V-E$ are as in Fig. 1.3.

We now introduce particular solutions of (0.1).

Let $x_1 \in \mathbb{C}$ be a point as in Fig. 1.3 which is above the Stokes lines starting from $\beta_+(E)$. We denote then by u a solution which increases exponentially from x_1 to $\alpha_+(E)$ and we put $\bar{u}(x,h)=\overline{u(\bar{x},\bar{h})}$.

Similarly $x_2 \in \mathbb{C}$ is a point as in Fig. 1.3 and we denote by v a solution which increases exponentially from x_2 to $\alpha_-(E)$, and we put $\bar{v}(x,h)=\overline{v(\bar{x},\bar{h})}$. In the symmetric case we take $v(x,h)=u(-x,h)$, and $x_2=-x_1$.

Using the results of Section 1, we see that we can take

$$u(x,h)=u_+(\alpha_+(E), x_1, x, h) \qquad \text{and} \qquad v(x,h)=u_-(\alpha_-(E), x_2, x, h)$$

for suitable choices of determination of $(V-E)^{1/2}$.

We will consider the unique solution of (0.1) (modulo a constant factor) denoted by u_0, which is in $L^2([0, +\infty[)$ and real on $\mathbb{R}$. The existence of u_0 is well known and follows from the hypotheses of Section 0. We cannot write u_0 directly using the results of Section 1, but we shall see later that on any bounded interval of $\mathbb{R}$, u_0 is close to functions of the type $u_-(\alpha_+(E), x_1, x, h)$, for x_1 big enough.

Finally, we denote by v_0 the unique solution of (0.1) in $L^2(]-\infty, 0])$ which is real on $\mathbb{R}$. In the symmetric case we will take $v_0(x, h) = u_0(-x, h)$.

If $\mathscr{L}$ is the linear space of solutions of (0.1), it is clear that $(u, \bar{u})$ and $(v, \bar{v})$ are two bases of $\mathscr{L}$. We have the following relations:

$$u_0 = cu + \bar{c}\bar{u}, \qquad v_0 = dv + \bar{d}\bar{v}, \qquad v = au + b\bar{u}, \qquad \bar{v} = \bar{b}u + \bar{a}\bar{u}.$$

Here a, b, c are given by

$$a = \frac{W(v, \bar{u})}{W(u, \bar{u})}, \qquad b = \frac{W(v, u)}{W(\bar{u}, u)}, \qquad c = \frac{W(u_0, \bar{u})}{W(u, \bar{u})}, \qquad d = \frac{W(v_0, \bar{v})}{W(v, \bar{v})}.$$

We have the following proposition:

PROPOSITION 2.1. *$E \in \mathbb{R}$ is an eigenvalue of $-h^2(d^2/dx^2) + V$ on $L^2(\mathbb{R})$ if and only if*

$$\frac{da + \bar{d}\bar{b}}{c} \quad \textit{is real.} \tag{2.1}$$

Proof. It is clear that E is an eigenvalue of $-h^2(d^2/dx^2) + V$ if and only if u_0 is collinear to v_0. Since $v_0 = (da + \bar{d}\bar{b})u + (\bar{d}\bar{a} + db)\bar{u}$ we immediatly get (2.1). ∎

Remark 2.1. In the symmetric case we see that $d = c$ so (2.1) becomes

$$a + \frac{\bar{d}b}{d} \quad \text{is real.}$$

We finally give some useful identities between the quantities a, b, c, d.

PROPOSITION 2.2. *The following identities hold:*

$$\textit{nonsymmetric case: } |b|^2 - |a|^2 = -\frac{W(v, \bar{v})}{W(u, \bar{u})}$$

$$\textit{symmetric case: } \begin{cases} |b|^2 - |a|^2 = 1 \\ a + \bar{a} = 0. \end{cases}$$

Proof. To prove the first identity we compute the matrix A of the change of basis from $(u, \bar{u})$ to $(v, \bar{v})$, and the inverse A^{-1}, using Wronskians between $u, \bar{u}, v$, and $\bar{v}$. Then the result follows from the fact that $AA^{-1} = Id$. In the symmetric case we consider the linear map S defined on $\mathscr{L}$ by $Sf(x) = f(-x)$. The matrix of S in the basis $(u, \bar{u})$ is $\left(\begin{smallmatrix} a & \bar{b} \\ b & \bar{a} \end{smallmatrix}\right)$. Since S is an involution different from $\pm Id$, we get the second identity. ∎

PROPOSITION 2.3. *Let* $\theta = \operatorname{Arg}((\bar{d}\bar{b})/c) - \pi/2$, $\alpha = \pi/2 + \operatorname{Arg}((ad)/c)$, *and* $\rho = |a/b|$. *Then the eigenvalue equation is equivalent to*

$$\cos\theta = \rho \cos\alpha. \tag{2.2}$$

In the symmetric case we get $\cos\theta = \rho$.

Proof. From Proposition 2.2 and Section 2.2 we see that ρ is less than 1.

It is then easy to get Proposition 2.3. ∎

2.2. *Computations of the Wronskians*

We now compute the Wronskians arising in Proposition 2.1.

Computation of $W(u_0, u)$: We first normalize u_0 such that $|u_0|_{L^2([0,+\infty[)} = 1$, and we take $x_3, x_4 \in \mathbb{R}^+$ such that $\alpha_+(E) < x_3 < x_4$, and x_3 is big enough. We can then write u_0 as

$$\begin{aligned} u_0 &= l_+(h)u_+(\alpha_+(E), x_3, x, h) + l_-(h)u_-(\alpha_+(E), x_4, x, h) \\ &= l_+(h)\tilde{u}_+ + l_-(h)\tilde{u}_-. \end{aligned} \tag{2.3}$$

Here we note that l_+, l_- are real, and we take the branch of $(V-E)^{1/2}$ which is positive on $[\alpha_+(E), +\infty[$. We get

$$\begin{aligned} \int_{x_3}^{x_4} |u_0|^2\,dx &= |l_+(h)|^2 \int_{x_3}^{x_4} |\tilde{u}_+|^2\,dx \\ &\quad + 2l_+(h)l_-(h)\int_{x_3}^{x_4} \tilde{u}_+\tilde{u}_-\,dx + |l_-(h)|^2 \int_{x_3}^{x_4} |\tilde{u}_-|^2\,dx. \end{aligned} \tag{2.4}$$

We can then use the results of Section 1, since we have asymptotic expansions for $\tilde{u}_+$ and $\tilde{u}_-$ valid uniformly in $[x_3, x_4]$.

We get

$$\int_{x_3}^{x_4} \tilde{u}_+\tilde{u}_-\,dx = O(1)$$

$$\int_{x_3}^{x_4} |\tilde{u}_+|^2\,dx \sim Ce^{+2z(x_3)/h}.$$

Since the left hand side of (2.4) stays bounded when h tends to zero, we get that

$$|l_+(h)| \leqslant Ce^{-z(x_3)/h}.$$

We now denote by $(V-E)_1^\alpha$ for $\alpha = \frac{1}{4}, \frac{1}{2}$ the branch of $(V-E)^\alpha$ positive for $x \in [\alpha_+(E), +\infty[$ extended continuously along Γ_1 (see Fig. 2.1). Then it is easy to see that we can take for u, defined at the beginning of the section, the function

$$u = u_+(\alpha_+(E), x_1, x, h).$$

Then $W(u_0, u) = l_+(h)\, W(\tilde{u}_+, u) + l_-(h)\, W(\tilde{u}_-, u)$. Using Proposition 1.1, we get $W(\tilde{u}_-, u) = (2/h)\psi_+(z_1, z_4, h)$, where $z_i = z(x_i)$. Using the same kind of arguments, we get

$$W(\tilde{u}_+, u) = -\frac{2}{h} e^{2z(x_1)/h} \varphi_+(z_3, z_1, h),$$

where $\varphi_+(z_3, z_1, h) \in O(h)$. If A is any positive real number, we see that

$$W(u_0, u) = \frac{2}{h} l_-(h)\, \psi_+(z_1, z_4 h) \text{ modulo } O(e^{-A/h}), \tag{2.5}$$

provided we take x_3 in (2.3) such that $z(x_3) - 2z(x_1) \geqslant A$.

In the sequel, we will forget the error term for simplicity of notation.

Computation of $W(u, \bar{u})$: For $\alpha = \frac{1}{2}, \frac{1}{4}$, we denote by $(V-E)_2^\alpha$ the branch of $(V-E)^\alpha$ positive on $[\alpha_+(E), +\infty[$ extended continuously along $\bar{\Gamma}_1$ (see Fig. 2.1). Then along Γ (see Fig. 2.1)

$$\begin{aligned} (V-E)_2^{1/2} &= -(V-E)_1^{1/2} \\ (V-E)_2^{-1/4} &= i(V-E)_1^{-1/4}. \end{aligned} \tag{2.6}$$

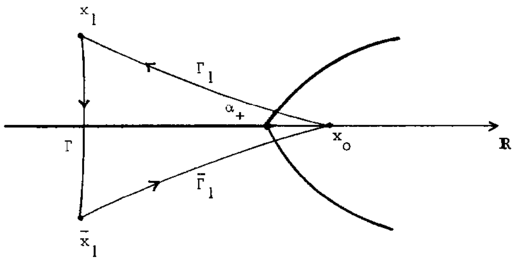


FIGURE 2.1

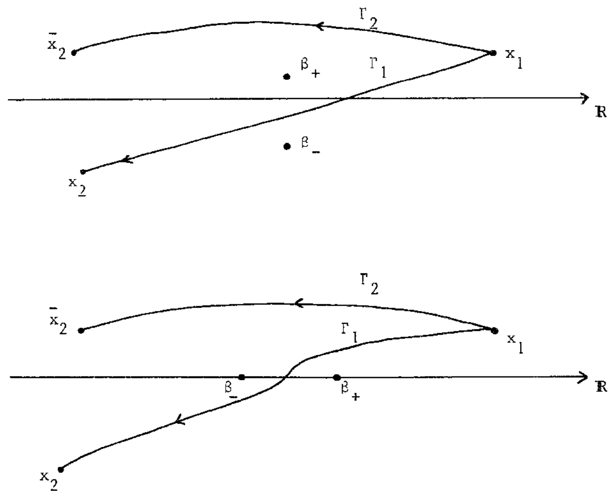


FIGURE 2.2

$\bar{u}$ can be written as $\bar{u}=u_+(\alpha_+(E), \bar{x}_1, x, h)$, where we now take the branch $(V-E)_2^{1/2}$. Using (2.6) we can also write

$$\bar{u}=iu_-(\alpha_+(E), \bar{x}_1, x, h),$$

where we now take the branch $(V-E)_1^{1/2}$. Using Proposition 1.1, we get

$$W(u, \bar{u})=-\frac{2i}{h}\psi_+(z_1, \bar{z}_1, h). \tag{2.7}$$

(Here by abuse of notation we put $\bar{z}_i=z(\bar{x}_i)$.) We note that $\psi_+(z_1, \bar{z}_1, h)$ is real.

Computation of $W(u, v)$: We denote again by $(V-E)_1^\alpha$ for $\alpha=\frac{1}{2}, -\frac{1}{4}$ the branch of $(V-E)^\alpha$ extended continuously along Γ_1 from x_1 to x_2 (see Fig. 2.2). We can write v as

$$v(x, h)=u_-(\alpha_-(E), x_2, x, h).$$

We can apply Proposition 1.1 if we notice that we used two different base points in $z(x)$, which amounts only to multiplying by a constant factor. We get

$$W(u, v)=-\frac{2}{h}\psi_+(z_1, z_2, h)\exp\left(\frac{1}{h}\int_{x_+(E)}^{\alpha_-(E)}(V-E)_1^{1/2}\,dt\right). \tag{2.8}$$

Here in the exponential, we integrate along Γ_1.

Computation of $W(u, \bar{v})$: We denote by $(V-E)_2^\alpha$ for $\alpha = \frac{1}{2}, -\frac{1}{4}$, the branch of $(V-E)^\alpha$ extended continuously from x_1 to $\bar{x}_2$ along the path Γ_2 on Fig. 2.2. We can write $\bar{v}$ as $\bar{v}(x, h) = -u_-(\alpha_-(E), \bar{x}_2, x, h)$, where we use the branch $(V-E)_2^{1/2}$. As in (2.8) we obtain

$$W(u, \bar{v}) = \frac{2}{h} \psi_+(z_1, \bar{z}_2, h) \exp\left(\frac{1}{h} \int_{\alpha_+(E)}^{\alpha_-(E)} (V-E)_2^{1/2}\, dt\right). \tag{2.9}$$

Computation of $W(v_0, v)$ *and* $W(v, \bar{v})$: It is easy to check that if we extend $(V-E)_1^\alpha$ along Γ_1 we get on $]-\infty, \alpha_-(E)]$ the branch of $(V-E)^\alpha$ which is positive there.

We can use the same arguments as in the computation of $W(u_0, u)$ except that v_0 will now be close to $u_+(\alpha_-(E), x_5, x, h)$ for x_5 large negative. Modulo an error term as in (2.5), we get

$$W(v_0, v) = -\frac{2}{h} m_-(h) \psi_+(z_5, z_2, h), \tag{2.10}$$

where $m_-(h)$ is defined like $l_-(h)$ (see (2.3)). Using the same arguments we also see that

$$W(v, \bar{v}) = \frac{2i}{h} \psi_+(z_2, \bar{z}_2, h). \tag{2.11}$$

2.3. *Action Integrals*

In this section we compute integrals of $(V-E)^{1/2}$ along some paths in the complex domain in order to complete formulas for the Wronskians given before. They are called action integrals because they are of the form $\pm i \int \xi\, dx$, where (x, ξ) belongs to the characteristic variety $\{\xi^2 + V(x) = E\}$. With the hypotheses given in Section 0, we can write

$$V(x) = -b^2(x), \tag{2.12}$$

with b real analytic, $b(0) = 0$, $b'(0) = (-V''(0)/2)^{1/2}$.

For $E < 0$ and small, the turning points $\beta_\pm(E)$ are real with

$$\beta_\pm(E) = \pm\left(\frac{2}{-V''(0)}\right)^{1/2} (-E)^{1/2}(1 + O(E)). \tag{2.13}$$

For $E < 0$ we define, by taking the positive square roots and integrating on the real line,

$$\begin{aligned} S(E) &= \int_{\beta_-}^{\beta_+} (V-E)^{1/2}\, dt \\ C_1(E) &= \int_{\beta_+}^{\alpha_+} (-V+E)^{1/2}\, dt \\ C_2(E) &= \int_{\alpha_-}^{\beta_-} (-V+E)^{1/2}\, dt. \end{aligned} \tag{2.14}$$

We see that all these quantities are positive, $S(E)$ is the Agmon distance between the two wells, and $C_i(E)$ is half of the area inside the characteristic variery $\{\xi^2 + V = E\}$ above the well $U_i(E)$.

We now define the continuous function of E,

$$\begin{aligned} C(E) &= C_1(E) + C_2(E) \qquad && E < 0 \\ C(E) &= \int_{\alpha_-}^{\alpha_+} (-V + E)^{1/2}\, dt \qquad && E \geqslant 0, \end{aligned} \tag{2.15}$$

and for $E > 0$, the negative function,

$$S(E) = \int_{\beta_-}^{\beta_+} (V - E)^{1/2}\, dt, \tag{2.16}$$

obtained by integrating on the segment joining β_- to β_+ and choosing the square root with a positive imaginary part.

We can now state:

PROPOSITION 2.3. *With the notation as above*

$$S(E) \text{ is an analytic function of } E \text{ near } 0, \qquad \text{with } S(0) = 0,$$
$$S'(0) = -\frac{\pi}{2}\left(\frac{2}{-V''(0)}\right)^{1/2}. \tag{2.17}$$

$$C(E) = A(E)\log(|E|) + B(E), \tag{2.18}$$

where A and B analytic functions of E near 0, with $A(E) = (1/\pi)S(E)$.

$$D(E) = C_1(E) - C_2(E) \tag{2.19}$$

defined for $E < 0$ extends as an analytic function of E near 0, vanishing identically if V is an even function.

Proof. We introduce the cycles γ and Γ as on Fig. 2.3, which are chosen such that β_+ and β_- stay inside γ for E small and similarly $\alpha_+, \alpha_-, \beta_+, \beta_-$ stay inside Γ.

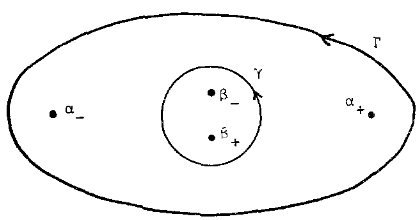


FIGURE 2.3

Γ and γ are independent of E and $\int_\gamma (V-E)^{1/2}\,dt$ and $\int_\Gamma (V-E)^{1/2}\,dt$ are obviously analytic functions of E.

It is easy to see that for good choices of the square roots we get

$$2S(E)=\int_\gamma (V-E)^{1/2}\,dt$$

$$2iD(E)=\int_\Gamma (V-E)^{1/2}\,dt.$$

This shows that $S(E)$ and $D(E)$ are analytic.

Now

$$S(E)=\frac{1}{2}\int_\gamma (-b^2(t)-E)^{1/2}\,dt=\frac{1}{2}\int_\gamma ib\left(1+\frac{E}{b^2}\right)^{1/2}\,dt.$$

Since we can choose γ such that b is holomorphic and nonvanishing on γ, we get for $|E|$ small enough

$$S(E)=\frac{i}{4}E\int_\gamma \frac{dt}{b(t)}+O(E^2)=-\frac{\pi}{2}\left(\frac{2}{-V''(0)}\right)^{1/2}E+O(E^2).$$

We now find the expression of $C(E)$:

The first step is to show that for $E>0$, $iC(E)$ is of the form indicated in the proposition. We consider the integral (for c real positive) $I(E)=\int_0^c (E-V(x))^{1/2}\,dx$ which is the singular part of $C(E)$.

It is then an elementary computation using the change of variables $t=b(x)$ to get the result.

We now compute $iC(e^{2i\pi}E)$ for $E>0$. The turning points near 0 are exchanged by the transformation $E\to e^{2i\pi}E$. The path of integration in (2.15) is transformed into the path drawn in Fig. 2.4. We get

$$iC(e^{2i\pi}E)=iC(E)-2S(E).$$

Hence $A(E)=(1/\pi)\,S(E)$, which shows (2.18) for $E>0$.

Now let $\tilde{C}(E)$ be the analytic extension of $C(E)$ in $E<0$ from the upper half plane.

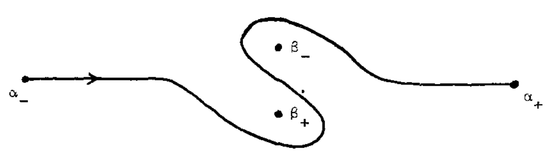


FIGURE 2.4

FIGURE 2.5

The path of integration in (2.15) is transformed into the path drawn on Fig. 2.5.

We get $\tilde{C}(e^{i\pi}E) = (1/\pi)\, S(-E)\log(E) + ((i\pi)/\pi)\, S(-E) = C(-E) + iS(-E)$ which proves (2.18) for $E < 0$. ▌

Using Proposition 2.3 we can rewrite (2.8) and (2.9) as

$$W(u, v) = \begin{cases} -\dfrac{2}{h} e^{-iC(E)/h} \psi_+(z_1, z_2, h) & \text{for} \quad E > 0 \\ -\dfrac{2}{h} e^{-iC(E)/h + S(E)/h} \psi_+(z_1, z_2, h) & \text{for} \quad E < 0 \end{cases} \tag{2.8$'$}$$

$$W(u, \bar{v}) = \begin{cases} \dfrac{2}{h} e^{-iD(E)/h + S(E)/h} \psi_+(z_1, \bar{z}_2, h) & \text{for} \quad E > 0 \\ \dfrac{2}{h} e^{-iD(E)/h + S(E)/h} \psi_+(z_1, \bar{z}_2, h) & \text{for} \quad E < 0. \end{cases} \tag{2.9$'$}$$

2.4. *Estimates as E Tends to Zero*

In this section we will estimate the symbols $\psi_+(z_1, z, h)$ computed above when E tends to 0.

From Figs. 2.1 and 2.2, it is clear that the symbols ψ_+ arising in $W(u_0, u)$, $W(u, \bar{u})$, $W(u, \bar{v})$, $W(v_0, v)$, and $W(v, \bar{v})$ are analytic in E near 0. The only difficult part is $\psi_+(z_1, z_2, h)$ which arises in $W(u, v)$ because the integration path gets pinched between the turning points $\beta_-(E)$ and $\beta_+(E)$, when E tends to zero.

We get the following proposition:

PROPOSITION 2.4. *For $|E| \geqslant C_1 h$ the following estimates hold uniformly*

$$\psi_+(z_1, z_2, h) = 1 + R(E, h) \qquad \textit{with} \quad R(E, h) \in O\left(\frac{h}{E}\right)$$

$$\frac{\partial}{\partial E} \psi_+(z_1, z_2, h) = \frac{\partial R}{\partial E} \qquad \textit{with} \quad \frac{\partial R}{\partial E} \in O\left(\frac{h}{E^2}\right).$$

Proof. Recall from Section 1 that if we put

$$I(f)(z) = \int_{z_1}^{z} e^{2(t_1 - z)/h} (H(t_1)\, f(t_1)\, dt_1)$$

and

$$J(f)(z)=\int_{z_1}^{z} H(t_1)\,f(t_1)\,dt_1$$

we have

$$\psi_+(z_1, z_2, h)=\sum_0^\infty W_{2p}(z_2, h) \qquad \text{and} \qquad W_{2p}=(J\circ I)^p(1).$$

Here the singularity in ψ_+ comes from the fact that on the integration path $z(\Gamma_1)$, H blows up like $1/(S(E))$ in a neighborhood of 0.

Let us denote by $z(E)$ the turning point $z(\beta_+(E))$.

The estimate given in Section 1.1 near a simple turning point shows that

$$\begin{aligned} |H(z)| &\leqslant \frac{C}{|z-z(E)|} \\ |H'(z)| &\leqslant \frac{C}{|z-z(E)|^2}. \end{aligned} \tag{2.20}$$

If we use Taylor's formula at $t_1=z$ to estimate $I(f)$ as in Proposition 1.2, we get

$$\begin{aligned} I(f)(z)=h\int_{(z_1-z)/h}^{0} e^{2s}Hf(z)\,ds + h^2\int_{(z_1-z)/h}^{0} e^s s\,ds \\ \times\int_0^1 (Hf)'(z+ths)\,dt. \end{aligned}$$

To estimate $J\circ I(f)$, we see that we must compute integrals of the form

$$\begin{aligned} I_1 &= \int_{z_1}^{z} |H(t_1)| \times |H(t_1+ths)|\,dt_1 \\ I_2 &= \int_{z_1}^{z} |H(t_1)| \times |H'(t_1+ths)|\,dt_1. \end{aligned}$$

Using Cauchy–Schwarz inequality, we are reduced to estimate

$$\int_{z_1}^{z} |H(t_1)|^2\,dt \qquad \text{and} \qquad \int_{z_1}^{z} |H'(t_1)|^2\,dt.$$

It is easy to see that near 0, $\operatorname{Re} z$ is zero on $z(\Gamma_1)$ and that $\operatorname{Re}(z-z(E))=\frac{1}{2}S(E)$.

The first integral is then of the type $\int_{z_1}^{z}(dt/(t_1^2+\frac{1}{4}S^2(E))$, and the second one is of the type $\int_{z_1}^{z}(dt_1/(t_1^2+\frac{1}{4}S^2(E))^2)$. We then easily get that $I_1 \leqslant C/|S(E)|$ and $I_2 \leqslant C/(S^2(E))$. Using these estimates we get

$$\sup |J \circ I(f)| \leqslant C_1 \left(\frac{h}{|S(E)|}+\left(\frac{h}{S(E)}\right)^2\right) \sup |f| + C_1 \frac{h^2}{|S(E)|} \sup |f'|.$$

On the other hand,

$$\frac{d}{dz}((J \circ I)(f)) = -\frac{2}{h} J \circ I(f) - HI(f).$$

If we put $\|g\| = \sup |g| + h \sup |g'|$, we first easily get that

$$\sup |I(f)| \leqslant C \frac{h}{|S(E)|} \sup |f|,$$

which gives

$$\|J \circ I(f)\| \leqslant C\left(\frac{h}{|S(E)|}\right) \|f\|,$$

if $h/|S(E)|$ is small enough. By taking $|E|$ bigger than $C_1 h$ for a suitable constant C_1, we can be sure that $C(h/|S(E)|) < \frac{1}{2}$ which proves the first part of the proposition.

To get the estimate of $(\partial/\partial E)\, \psi_+(z_1, z_2, h)$, we remark that $|\partial H/\partial E| \leqslant C/|z-z(E)|^2$. We can use the same method as above to estimate $(\partial/\partial E) J \circ I(f)$ in terms of $(\partial/\partial E) f$. ∎

Remark 2.2. If we make the change of variables $x = h^{1/2} t$ in Eq. (0.1), we see easily that the Wronskian $W(u, v)$ is an analytic function of h and E/h near 0. This shows that in fact the singularities of $C(E)/h$ and of $\psi_+(z_1, z_2, h)$ in $W(u, v)$ cancel out for E/h small, so the representation of the Wronskian with phase and amplitude is no more useful in this case.

3. Proof of the Theorems

We first introduce some notation. S_a^k will be the space of analytic symbols $a(E, h)$ of order k in h (see [Sj]). We will say that a function $m(E, h)$ is in S_a^k if m is asymptotic to an analytic symbol in S_a^k when h tends to zero.

3.1. *Estimation of Eigenvalue Splitting*

We assume that V is even. In the region $E < 0$, it is well known that the eigenvalues of P come out in pairs with exponentially small splittings (see [HSj, Si] and references there).

We get the following theorem:

THEOREM 3.1. *For $-\varepsilon_1 < E < -\varepsilon_0$, where ε_1 is small enough, if $E_+(h)$ and $E_-(h)$ are a pair of eigenvalues exponentially close to the energy level E, the splitting is of the form*

$$E_+ - E_- = m(E, h)\, e^{-S(E)/h} + O(e^{-2S(E)/h}),$$

where $m(E, h) \in S_a^{-1}$, and

$$m(E, h) = \frac{2h}{T_E} + O(h^2),$$

where T_E is the period of the Hamiltonian flow on $\{p = E\}$.

Proof. In the symmetric case, d is equal to c and

$$\frac{\bar{b}\bar{d}}{c} = -\frac{\overline{W(v, u)}}{W(u, \bar{u})} \times \frac{W(u_0, u)}{W(u_0, \bar{u})}.$$

$(W(u_0, u))/(W(u_0, \bar{u}))$ is of modulus one and equal to 1 modulo $O(h)$, so we get

$$\frac{W(u_0, u)}{W(u_0, \bar{u})} = e^{i\theta_1(E,h)} \qquad \text{with} \quad \theta_1 \in S_a^{-1}$$

$$\bar{b} = \frac{\overline{W(v, u)}}{W(u, \bar{u})} = e^{iC(E)/h + S(E)/h} \frac{\bar{\psi}_+(z_1, z_2, h)}{-i\psi_+(z_1, \bar{z}_1, h)} = i \times e^{iC(E)/h + S(E)/h}(1 + O(h)).$$

We get $\theta = -\pi + C(E)/h + \theta_2(E, h)$ with $\theta_2 \in S_a^{-1}$. Since $c = d$ and a is pure imaginary (see Proposition 2.2), we get $\alpha = 0$. Finally, $\rho = |a/b| = (1 - |b|^{-2})^{1/2} = 1 - \frac{1}{2}k(E, h)\, e^{-2S(E)/h} + O(^{-4S(E)/h})$ where $k(E, h) \in S_a^0$ and $k = 1 + O(h)$. Let $E_0(h)$ be a solution of $\cos(\theta(E, h)) = -1$. Then the two solutions of (3.2) near E_0 are given by

$$\theta(E, h) - \theta(E_0, h) = \pm(k)^{1/2}\, e^{-S(E)/h} + O(e^{-2S(E)/h}).$$

Using a well-known result from classical mechanics, we know that $C'(E) = T_E$, where T_E is the period of the Hamiltonian flow on the energy surface $\{p = E\}$. Then we get

$$E_+ - E_- = m(E, h)\, e^{-S(E)/h} + O(e^{-2S(E)/h}).$$

Using Appendix A.2, we know that $m(E, h)$ is asymptotic to an analytic symbol of order -1, and

$$m(E, h) = \frac{2h}{T_E} + O(h)^2. \quad ∎$$

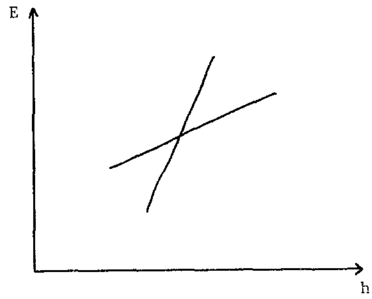


FIGURE 3.1

Remark 3.1. This first term was already written in Landau–Lifchitz's "Quantum Mechanics," Chapter VII.

3.2. *Nearly Avoided Crossings of Eigenvalues*

We consider now the nonsymmetric case. In this situation, it is well known that the spectrum of P is exponentially close to the union of the spectra of P restricted to each of the two potential wells U_1 and U_2 (for example, by use of suitable Dirichlet problems). As we shall see in the proof of Theorem 3.2, these spectra are given by W.K.B. approximations,

$$\begin{aligned} C_1(E) + h\theta_1(E, h) &= \left(\frac{\pi}{2} + k_1\pi\right) h + O(h^\infty) \qquad \text{for } U_1 \\ C_2(E) + h\theta_2(E, h) &= \left(\frac{\pi}{2} + k_2\pi\right) h + O(h^\infty) \qquad \text{for } U_2, \end{aligned} \tag{3.1}$$

with $\theta_1, \theta_2 \in S_a^{-1}$. If we let h vary and follow a pair of W.K.B. eigenvalues, we get the result shown in Fig. 3.1.

However, since in one dimension the eigenvalues are simple, the true situation is shown in Fig. 3.2.

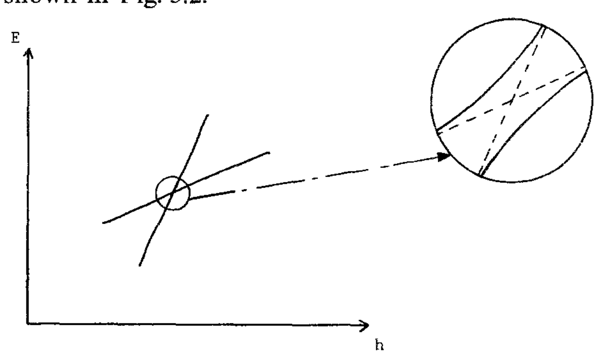


FIGURE 3.2

We will now estimate the difference between the true eigenvalues when the W.K.B. approximations coincide.

THEOREM 3.2. *Let h_0 and $E_0(h_0)$ with $-\varepsilon_1 < E_0 < -\varepsilon_0$ be an energy level where the W.K.B. approximations for each well coincide. Then the smallest difference between the two eigenvalues of P near E_0 is equal to*

$$E_+ - E_- = m(E_0, h_0)\, e^{-S(E_0)/h_0} + O(e^{-2S(E_0)/h_0}),$$

where $m(E, h) \in S_a^{-1}$, and

$$m(E, h) = \frac{2h}{(T_{1E} T_{2E})^{1/2}} + O(h^2),$$

where T_{iE} is the period of the Hamiltonian flow on $\{p = E\}$ above U_i.

Proof. We first write the eigenvalue Eq. (3.2) in the nonsymmetric case:

$$\frac{d\bar{b}}{c} = \frac{\overline{W(v, u)}}{W(v, \bar{u})} \frac{W(v_0, v)}{W(\bar{v}, v)} \frac{W(u, \bar{u})}{W(u_0, \bar{u})}.$$

Using (2.5)–(2.11), we see that

$$\frac{W(v_0, v)\, W(u, \bar{u})}{W(\bar{v}, v)\, W(u_0, \bar{u})} = (-1 + O(h)) \frac{m_-(h)}{l_-(h)}$$

so that

$$\operatorname{Arg}\left(\frac{W(v_0, v)\, W(u, \bar{u})}{W(\bar{v}, v)\, W(u_0, \bar{u})}\right) = \pi + \theta_1(E, h) \qquad \text{with } \theta_1 \in S_a^{-1};$$

$$\bar{b} = \frac{\overline{W(v, u)}}{W(v, \bar{u})} = e^{i(C_1(E) + C_2(E))/h + S(E)/h} \frac{\bar{\psi}_+(z_1, z_2, h)}{-i\psi_+(z_1, \bar{z}_1, h)},$$

so we get

$$\theta = -\pi + (C_1(E) + C_2(E))/h + \tilde{\theta}_2(E, h) \qquad \text{with } \tilde{\theta}_2 \in S_a^{-1}$$

$$\frac{ad}{c} = \frac{W(v, \bar{u})}{W(u, \bar{u})} \frac{W(v_0, u)}{W(v, \bar{v})} \frac{W(u, \bar{u})}{W(u_0, \bar{u})}.$$

Using the same arguments, we get $\alpha = (C_1 - C_2)/h + \tilde{\theta}_3(E, h)$, with $\tilde{\theta}_3 \in S_a^{-1}$. Finally,

$$\rho = \left|\frac{a}{b}\right| = \left(1 + \frac{W(v, \bar{v})}{W(u, \bar{u})} |b|^{-2}\right)^{1/2}$$

$$= 1 - \frac{1}{2} k(E, h)\, e^{-2S(E)/h} + O(e^{-4S(E)/h}),$$

where $k(E, h) \in S_a^0$ and $k = 1 + O(h)$.

If we look only for W.K.B. approximations of eigenvalues, we can forget the exponentially small error and put $\rho = 1$. We get the equation $\cos((C_1 + C_2)/h + \tilde{\theta}_2) = -\cos((C_1 - C_2)/h + \tilde{\theta}_3)$. If we put $\theta_1 = (\tilde{\theta}_2 + \tilde{\theta}_3)/2$ and $\theta_2 = (\tilde{\theta}_2 - \tilde{\theta}_3)/2$, we get $\cos(C_1/h + \theta_1) \times \cos(C_2/h + \theta_2) = 0$. We recover the formulas (3.1).

Now let $E_0(h_0)$ be an energy level where the two W.K.B. approximations for each well coincide, i.e., E_0 satisfies

$$C_i(E_0) + h_0 \theta_i(E_0, h_0) = (\pi/2 + k_i \pi) h_0 \qquad \text{for} \quad i = 1, 2.$$

We now compute the two true solutions of (2.2) near E_0. If we define δ_i by

$$C_i(E) + h\theta_i(E, h) = h\delta_i(E, h) + (\pi/2 + k_i \pi) h, \tag{3.2}$$

we easily transform (2.2) in

$$\tan(\delta_1) \tan(\delta_2) = \frac{1-\rho}{1+\rho}. \tag{3.3}$$

Using again that $C_i'(E) = \frac{1}{2} T_{iE}$, where T_{iE} is the period of the Hamiltonian flow on the energy surface $\{p = E\}$ above U_i, we get

$$\tfrac{1}{4} T_{1E} T_{2E} (E - E_0)^2 = \tfrac{1}{4} k(E, h)\, e^{-2S(E)/h} (1 + O(e^{-4S(E)/h}) + O(E - E_0)^2).$$

So the smallest difference between the two solutions near E_0 is equal to

$$E_+ - E_- = m(E, h)\, e^{-S(E)/h} + O(e^{-2S(E)/h}).$$

We know from Appendix A.2 that $m(E, h)$ is asymptotic to an analytic symbol of order -1, and we see that

$$m(E, h) = \frac{2h}{(T_{1E} T_{2E})^{1/2}} + O(h^2).$$

This completes the proof. ∎

Remark 3.2. It is clear that the results of Theorems 3.1 and 3.2 still hold for $E < -\varepsilon_1$, provided the geometry of the turning points of $V - E$ near the wells stays the same.

Remark 3.3. In the region $E > \varepsilon_0 > 0$, we can recover the results of [HR]. Namely, in this case (3.2) easily gives

$$\cos(-\pi + C(E)/h + \theta_1(E, h)) = \rho \cos \alpha,$$

where $\theta_1 \in S_a^{-1}$ and $\rho = O(e^{-S(E)/h})$. We get

$$C(E) + h\theta_1(E, h) = \left(\frac{\pi}{2} + k\pi\right) h + O(e^{-S(E)/h})$$

and solutions $E(h)$ are analytic symbols in h.

3.3. *Eigenvalues near the Top of the Barrier*

We now look at the transition between the zones $E > \varepsilon_0$ and $E < -\varepsilon_0$. We will be able to say something about the eigenvalues of P in the zone $|E| \geqslant C_1 h$, for some constant C_1 depending on the potential V. We will assume for simplicity that V is even. We call E an even (resp. odd) eigenvalue if E is associated with an even (resp. odd) eigenfunction.

To study the transition between the two zones, we will by $E = E_0^+$ an even eigenvalue, by E_0^-, E_1^+ the two next eigenvalues of P which are respectively odd and even. We have $E_0^+ < E_0^- < E_1^+$. Then we can measure the coupling of the eigenvalues by comparing $\frac{1}{2}(E_1^+ - E_0^+)$ and $(E_0^- - E_0^+)$. In the zone $E > \varepsilon_0$ these two numbers are equal modulo $O(h^2)$ and we have no coupling.

In the zone $E < -\varepsilon_0$, $\frac{1}{2}(E_1^+ - E_0^+)$ is of the order of Ch and $E_0^- - E_0^+$ is $O(e^{-S(E)/h})$ and we have a strong coupling. The transition is described in the following theorem:

THEOREM 3.3. *When E stays in the zone $|E| \geqslant C_1 h$*

$$\frac{1}{2}(E_1^+ - E_0^+) = \frac{\pi C_0 h}{\log E} + O\left(\frac{h}{\log^2 E}\right)$$

$$E_0^- - E_0^+ = \frac{2C_0 h}{\log E} \operatorname{arc\,tan}(e^{-S(E)/h}) + O\left(\frac{h}{\log^2 E}\right)$$

uniformly when E and h tend to zero. Here $C_0 = 2(-V''(0)/2)^{1/2}$.

Proof. It is easy to see that the eigenvalue Eq. (2.2) is equivalent to $a - ((bc)/\bar{c}) = \pm 1$. The plus sign corresponds to an odd eigenvalue and the minus sign to an even eigenvalue.

We then get that in (3.2) a solution E is an odd (resp. even) eigenvalue if $\theta(E)$ is positive (resp. negative). We can follow the proof of Theorem 3.1. The only difference is that the argument of $\bar{\psi}(z_1, z_2, h)$ is no longer an analytic symbol of order -1, when E tends to 0. Using Proposition 2.4, we get instead $\arg(\bar{\psi}_+(z_1, z_2, h)) = K(E, h)$ with

$$\left.\begin{aligned} &K(E, h) \in O\left(\frac{h}{E}\right) \\ &\frac{\partial K}{\partial E} \in O\left(\frac{h}{E^2}\right). \end{aligned}\right. \qquad \text{(uniformly for } |E/h| \leqslant C_1) \qquad (3.4)$$

We get $\theta = -\pi + C(E)/h + K(E, h) + \theta_1(E, h)$ with $\theta_1 \in S_a^{-1}$. As in Theorem 3.1, we get $\alpha = 0$ and $\rho = |a|/(1+|a|^2)^{1/2} = \cos(\pi/2 - \arc\tan(|a|))$:

$$|a| = (1 + O(h))\, e^{(S(E)/h)}, \tag{3.5}$$

where the $O(h)$ is uniform when E tends to zero. Here it is important to notice that $e^{S(E)/h}$ is neither exponentially big nor exponentially small when E/h is bounded.

Equation (3.2) becomes $\cos(-\pi + C(E)/h + \theta_1(E, h) + K(E, h)) = \cos(\pi/2 - \arc\tan(|a|))$. We get two solutions

$$C(E) + h\theta_1 + hK = (\pi/2 + (2k+1)\pi)h - h \arc\tan(|a|) \qquad \text{(odd eigenvalue)}$$

$$C(E) + h\theta_1 + hK = (-\pi/2 + (2k+1)\pi)h + h \arc\tan(|a|) \quad \text{(even eigenvalue).}$$

Let $E_0^+ = E$ be an eigenvalue of P.

E_0^+ is the solution of $C(E) + h\theta_1 + hK = ((2k+1)\pi - \pi/2)h + h \arc\tan(|a|)$. The next odd eigenvalue of P is the solution E_0^- of

$$C(E) + h\theta_1 + hK = ((2k+1)\pi + \pi/2)h - \arc\tan(|a|).$$

The next even eigenvalue of P is the solution E_1^+ of

$$C(E) + h\theta_1 + hK = ((2k+1)\pi - \pi/2)h + 2\pi h + h \arc\tan(|a|).$$

Using (3.4) and (3.5) we see that $(\partial/\partial E)(hK)$ and $(\partial/\partial E)(h \arc\tan(|a|))$ are $O(1)$ uniformly in $|E| \geqslant C_1 h$.

We can then use Newton's method to estimate the differences $E_0^- - E_0^+$ and $E_1^+ - E_0^+$, since $C'(E) = \frac{1}{2}(2/(-V''(0)))^{1/2} \log E + O(1)$. We get

$$E_1^+ - E_0^+ = \frac{2C_0 h}{\log E} + O\left(\frac{h}{\log^2 E}\right)$$

$$E_0^- - E_0^+ = C_0 h \left(\frac{\pi - 2 \arc\tan(e^{S(E)/h}(1 + O(h))}{\log E}\right)\left(1 + O\frac{1}{\log(E)}\right)\right)$$

which proves the theorem. ∎

Remark 3.4. It is possible to study the weak coupling near the top of the barrier in the noneven case. In the zone $|E| > C_1 h$ we get

$$\cos(-\pi + C(E)/h + \theta_1(E, h) + K(E, h)) = \rho \cos \alpha$$

with $\rho = \pi/2 - \arc\tan(e^{S(E)/h})$ approximately and $\alpha = D(E)/h + \theta_2(E, h)$. Since $S(E)$ and $D(E)$ are analytic functions of E as seen in Section 2.3 their derivatives are bounded near $E=0$. If we denote $E_0^+ < E_0^- < E_1^+$ successive eigenvalues as above we see that we still have

$$\frac{1}{2}(E_1^+ - E_0^+) = \frac{\pi C_0 h}{\log E} + O\left(\frac{h}{\log^2 E}\right),$$

but $E_0^- - E_0^+$ is oscillating between the values

$$\frac{C_0 h}{\log E}\left(\pi \pm 2 \arctan(e^{S(E)/h}(1+O(h)))\left(1 + O\frac{1}{\log(E)}\right)\right).$$

Remark 3.5. When E varies between ε_0 and $C_1 h$, $e^{-S(E)/h}$ varies approximately between $e^{-S(\varepsilon_0)/h}$ and $e^{-\pi C_1/C_0}$. We see a limited coupling of the eigenvalues at a distance $C_1 h$ from the top of the barrier. On the other side of the barrier, when E is equal to $-C_1 h$, $e^{-S(E)/h}$ is already of the size of $e^{-\pi C_1/C_0}$ so the eigenvalues are very strongly coupled as soon as C_1/C_0 is bigger than 1. We believe that the number of eigenvalues in the zone $|E| \leqslant C_1 h$ is uniformly bounded in h, as h tends to zero.

This problem was studied in [FHWW] when V is equal to $-\frac{1}{2}x^2$ near 0 using special functions. However, their use of Newton's method for E/h small seems unjustified.

Remark 3.6. It is possible to relax the hypotheses about V. For example, we assume that V is only C^∞ outside a neighborhood of the wells. The representation formulas obtained for u_0 and v_0 still hold if we integrate on the real line in (1.4).

Remark 3.7. It is also possible to get results on eigenvalues and eigenfunctions of Dirichlet problems which could be applied to multiple wells in the spirit of [HSj]. If $x_0 \in \mathbb{R}$ is a point outside the potential well, we denote by u_d the solution of (0.1) with $u_d(x_0)=0$. Using the notations of 2.2, we take $x_3 < x_0 < x_4$ and we get

$$u_d = l_+ \tilde{u}_+ + l_- \tilde{u}_-.$$

If we normalize u_d such that $l_- = 1$, we easily get that $l_+ = O(e^{-2d(U,x_0)/h})$ where $d(U, x_0)$ is the Agmon distance from x_0 to the well $U(E)$. The rest of the argument is then straightforward.

Appendix

A.1. *Transport Equations*

We prove the assertion in the proof of Proposition 1.2. This result can be easily obtained using the general theory of [Sj] (see, for example, Theorem 9.3 of [s_j]).

Recall first that an expansion $a(x, h) = \sum_0^\infty a_k(x) h^k$ is an analytic symbol if $|a_k(x)| \leqslant C^k k^k$ for some constant C. For completeness we give a short proof using the ideas there.

Let $\Omega = \{x \in \mathbb{C} \mid |x| < r\}$ and for $0 < t \leqslant r$, $\Omega_t = \{x \in \mathbb{C} \mid |x| \leqslant r - t\}$.

Let $a(x, h) = \sum_0^\infty a_k(x) h^k$ be a symbol such that the a_k are analytic in Ω and satisfy the estimates

$$\sup_{\Omega_t} |a_k| \leqslant \frac{f(a, k)}{t^k} k^k \qquad \text{for} \quad 0 < t \leqslant r; \tag{A.1}$$

we say that a is an analytic symbol if for μ small enough the sum $\sum_0^\infty f(a, k) \mu^k$ is convergent. Here $f(a, k)$ are the best constants in (A.1). We introduce a norm on the vector space A_Ω of analytic symbols by putting

$$\|a\|_\mu = \sum_0^\infty f(a, k) \mu^k.$$

We now estimate the norms of the operators $(\partial_x)^{-1}$ and $h\partial_x$, where $(\partial_x)^{-1} a$ is the primitive of a vanishing at 0. It is easy to see that

$$\sup_{\Omega_t} |\partial_x^{-1} a_k| \leqslant \frac{f(a, k)}{(k-1) t^{k-1}} k^k,$$

so we get

$$\|\partial_x^{-1}\|_{\mathscr{L}(A_\Omega, A_\Omega)} \leqslant C_0.$$

We now estimate the norm of $h\partial_x$; the Cauchy formula gives

$$\partial_x b_k(z) = \frac{1}{2\pi i} \int_\Gamma \frac{b_k(t)}{(t-z)^2} \, dt.$$

If $z \in \Omega_t$ and we integrate on a circle of radius $C \times (t - s)$, we get

$$\sup_{\Omega_t} |\partial_z b_k| \leqslant \frac{C}{t-s} \sup_{\Omega_s} |b_k| \leqslant \frac{C f(b, k)}{(t-s) s^k} k^k.$$

We now take the best possible s in this estimate, and we get:

$$\sup_{\Omega_t} |\partial_z b_k| \leqslant \frac{C f(b, k)}{t^{k+1}} (k+1)^{k+1}.$$

This immediately gives

$$\|h\partial_x\|_{\mathscr{L}(A_\Omega, A_\Omega)} \leqslant C_1 \mu. \tag{A.2}$$

We can now prove the proposition.

Recall that the $W_{n,\pm}$ are solutions of Eqs. $(1.3)_\pm$. We consider only the $+$ case.

Assume that W_{2p-1} is an analytic symbol. Then we know from the estimates above that

$$\|W_{2p}\|_\mu \leqslant C_0 \, \|W_{2p-1}\|_\mu,$$

since multiplication by H is obviously a bounded operator.

Using the other equation we get

$$W_{2p+1} + h\partial_z(W_{2p+1}) = \frac{h}{2} HW_{2p}.$$

We can solve this equation by a Neumann series,

$$W_{2p+1} = \sum_{k=0}^{\infty} (-1)^k (h\partial_z)^k \left(\frac{h}{2} HW_{2p}\right),$$

provided μ is small enough. We get

$$\|W_{2p+1}\|_\mu \leqslant C\mu \, \|W_{2p}\|_\mu.$$

This easily implies the convergence in A_Ω of the sums $\sum_0^\infty W_{2p}$ and $\sum_0^\infty W_{2p+1}$, which proves the proposition.

A.2. *Implicit Function Theorem*

We prove here the assertion in the proof of Theorem 3.1.

We assume that $a(E, h) = a_0(E) + ha_1(E) + \cdots$ belongs to A_Ω and that $a_0(0) = 0$, $a_0'(0) \neq 0$. As above we define the Banach space A to be the space of symbols $a = \sum_0^\infty a_k k^k h^k$ such that for μ small enough

$$\|a\|_\mu = \sum_0^\infty a_k \mu^k \qquad \text{is finite.}$$

We want to solve in E the equation

$$a(E, h) = 0. \tag{A.3}$$

One has $a(E, h) = a_0'(0)E + E^2 \times b(E) + h \times a_1(E, h)$. Solving (A.3) is equivalent to finding a fixed point for the nonlinear operator

$$R\colon E \to \frac{b(E)E^2}{-a_0'(0)} + \frac{ha_1(E, h)}{-a_0'(0)}.$$

It is then easy to see that R is a contraction on the ball $\{a \mid \|a\|_\mu \leqslant \varepsilon\}$ if ε and μ are small enough, so we can apply the fixed point theorem to prove the assertion.

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